

Monte Carlo Sampling in Fractal Landscapes

Jorge C. Leitão,^{1,2,*} João M. Viana Parente Lopes,^{3,†} and Eduardo G. Altmann^{1,‡}

¹Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

²CFP and Faculdade de Ciências da Universidade do Porto, 4169-007 Porto, Portugal

³CEsA - Centre for Wind Energy and Atmospheric Flows and

Faculdade de Engenharia da Universidade do Porto, 4200-465 Porto, Portugal

(Dated: February 20, 2013)

We propose a flat-histogram Monte Carlo method to efficiently sample fractal landscapes such as escape time functions of open chaotic systems. This is achieved by using a random-walk step which depends on the height of the landscape via the largest Lyapunov exponent of the associated chaotic system. By generalizing the Wang-Landau algorithm, we obtain a method which simultaneously constructs the density of states (escape time distribution) and the correct step-length distribution. As a result, averages are obtained in polynomial computational time, a dramatic improvement over the exponential scaling of traditional uniform sampling. Our results are not limited by the dimensionality of the phase space and are confirmed numerically for dimensions as large as 30.

PACS numbers: 05.10.Ln, 05.45.Df, 05.45.Pq, 02.07.Uu

The development of Monte Carlo methods had a dramatic impact on our understanding of high-dimensional systems. The spectrum of applications of these methods was considerably expanded with the development of optimized methods, such as flat-histogram [1–3] and parallel tempering [4], and now-a-days includes problems in a variety of fields, ranging from fluid dynamics [5] and spin systems [1–3] to protein simulations [6, 7]. These methods efficiently compute averages using non-uniform sampling and are optimized to problems on which the high dimensionality of the system leads to phase spaces with rough and complex energy landscapes.

In chaotic dynamical systems, complex landscapes appear even in low dimensions due to the sensitivity of initial conditions. Prominent examples of such landscapes appear in open systems showing chaotic transients. Transient chaos is a classical problem of nonlinear dynamics [8] with recent applications in fields ranging from quantum scattering to chemical and biological reactions in fluid flows [9, 10]. In open chaotic systems, the number of trajectories with escape time t decays as $\rho(t) \sim e^{-\kappa t}$ (κ is the escape rate) and the $t = \infty$ trajectories build a uncountable fractal set. The dependence of t on the phase-space variables \mathbf{r} build thus a fractal landscape as the one illustrated in Fig. 1. This example of extreme rough landscape poses major numerical challenges [9]. While algorithms beyond uniform sampling have been proposed for specific problems, e.g. to compute the fractal dimension [11] or to find long-living trajectories [12–14], there is still no general framework to sample the phase space of such systems.

In this paper we show how Monte Carlo methods can be applied to fractal landscapes such as those appearing in open chaotic systems. The crucial step is to design a random walk able to explore the extreme roughness of fractal landscapes. We show that an efficient flat-histogram simulation is only obtained using a random-

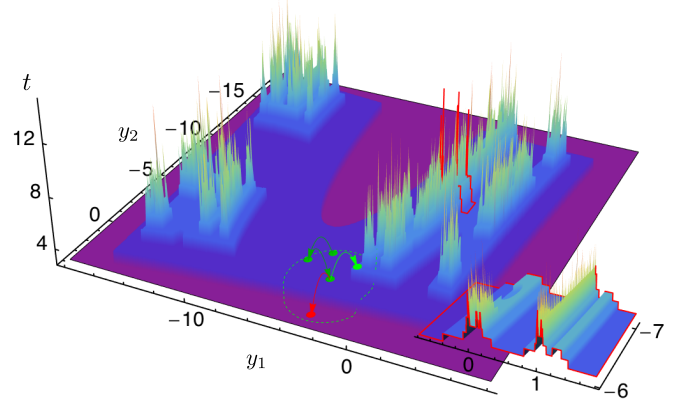


FIG. 1: (Color online) Fractal landscapes appear in the escape time function of open chaotic systems. Escape time t as a function of the phase space coordinates (y_1, y_2) at $x_1 = x_2 = 0$ of the 4-Dimensional coupled Hénon maps defined in Eq. (6). Inset: magnification of the red rectangle showing a Cantor-set-like profile. The circles (states) and arrows (proposals) represent the random walk (green/red indicate accepted/rejected proposals) underlying the Monte Carlo sampling.

walk step length σ which scales with the landscape height t as $\sigma(t) \sim e^{-\lambda_L t}$, where λ_L is the maximum Lyapunov exponent of the underlying chaotic system. Moreover, by extending the Wang-Landau procedure [2] to the proposal distribution, we obtain an adaptive algorithm which provides simultaneously $\rho(t)$ and $\sigma(t)$. In open chaotic systems, our approach changes the scaling of the computational effort from exponential to polynomial with the maximum escape time and both efficiently finds the large t trajectories and computes averages over the phase space.

We consider a fractal landscape as an escape time function of a transient chaotic system. Given a discrete-time open dynamical system $\mathbf{r}_{t+1} = \mathbf{F}(\mathbf{r}_t)$ defined in a D di-

mensional phase space Ω , the escape time $t(\mathbf{r})$ is defined as the number of iterations needed for an initial condition \mathbf{r} to leave the region of non-trivial dynamics [9]. We propose an algorithm that constructs both the total volume $\rho(t)$ of the landscape and the optimal proposal width $\sigma(t)$ at each t , in a predetermined *time-spectrum* $[t_{\min}, t_{\max}]$ and with a precision f which is successively reduced (initially $f = e$ and $\sigma(t) = \rho(t) = 1$ for all t). We consider a state dependent random walk in the space of initial conditions $\Gamma \in \Omega$ [25] initialized at $\mathbf{r} \in \Gamma, t = t(\mathbf{r})$, which evolves according to the following four steps:

- S1-** propose a state $\mathbf{r}' \in \Gamma$ with $t' = t(\mathbf{r}') \in [t_{\min}, t_{\max}]$ [e.g., using Eq. (1) below].
- S2-** accept/reject the state according to flat-histogram choice [Eq. (5) below].
- S3-** update $\rho(t)$ and $\sigma(t)$ as:
 - S3.1-** $\rho(t) \leftarrow \rho(t)f$ (Wang-Landau);
 - S3.2-** $\sigma(t) \leftarrow \sigma(t)f$ if $t' = t$; $\sigma(t) \leftarrow \sigma(t)/f$ if $t' < t$.
- S4-** After a number of repetitions of **S1-S3**, refine $f \leftarrow \sqrt{f}$ and go to **S1**.

After the convergence ($f = f_{\min} \gtrsim 1$), the random walk corresponds to a flat-histogram Monte Carlo simulation on t [1] (using only **S1** and **S2**). We now describe in more detail the steps **S1-S4**.

S1-Proposal - The ideal proposal should be able to explore the order of the landscape for an efficient search. In discrete spaces, often considered in spin systems, there is a natural local proposal given by flipping a single spin [15]. In continuous spaces the locality of the proposal is determined by the neighborhood around the present state. Fractal landscapes do not have a global characteristic length scale [8, 9] and therefore we consider a time dependent proposal width $\sigma = \sigma(t)$. Accordingly, we choose the conditional probability of proposing a new state \mathbf{r}' given \mathbf{r} as

$$g(\mathbf{r} \rightarrow \mathbf{r}') = \hat{\mathbf{u}} \frac{1}{\sigma(t(\mathbf{r}))} e^{-|\mathbf{r}-\mathbf{r}'|/\sigma(t(\mathbf{r}))} , \quad (1)$$

where $\hat{\mathbf{u}}$ is a random vector on the surface of the D-dimensional unit-hypersphere, and $\sigma(t)$ gives the characteristic length of the distribution [26].

We now show how $\sigma(t)$ has to scale with t for an efficient proposal. We consider the construction of the Cantor set [8, 9] as a paradigm of fractal landscape, see Fig. 2. The construction starts by splitting the interval $[0, 1]$ in the intervals $[0, 1/a]$, $[1/a, 1 - 1/b]$, $[1 - 1/b, 1]$ and assigning the escape time $t = 0$ to the middle interval (plateau at $t = 0$). This procedure is repeated on each of the 2 surviving intervals by assigning $t = 1$ to each of their 2 middle intervals (plateaus at $t = 1$), and again in the remaining intervals *ad infinitum*. In

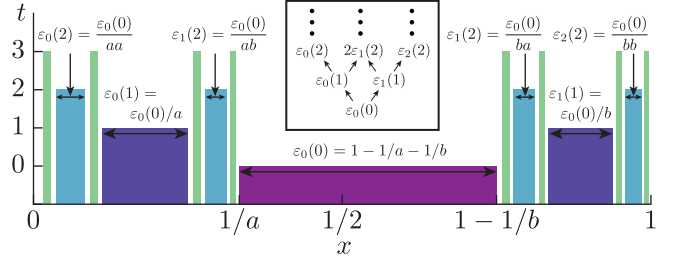


FIG. 2: (Color online) The construction of the 2-scale Cantor set with scales $1/a$ and $1/b$ as a paradigmatic fractal landscape. A plateau at t with width $\varepsilon(t)$ generates two plateaus at $t+1$, with widths $\varepsilon(t+1) = \varepsilon(t)/a$ and $\varepsilon(t+1) = \varepsilon(t)/b$, as indicated in the inset. At each t , the 2^t plateaus have lengths $\varepsilon_k(t)$ with $k = 0 \dots t$.

order to achieve an efficient proposal we have to know the scaling of the typical length of the plateaus $\tilde{\varepsilon}(t)$ with t . For the 1-scale Cantor set ($a = b$), each of the 2^t plateaus have a unique length given by $\varepsilon(t) = (1 - 2/a)(1/a)^t$ and thus $\tilde{\varepsilon}(t) = \varepsilon(t)$. For the 2-scale Cantor set ($a \neq b$), the 2^t plateaus have $t+1$ different lengths $\varepsilon_k(t) = (1 - 1/a - 1/b)(1/a)^{t-k}(1/b)^k$ with $k = 0, \dots, t$ and the number of plateaus with size $\varepsilon_k(t)$ is the binomial coefficient $B(t, k)$, see inset of Fig. 2. The total length at t is $\rho(t) = (1 - 1/a - 1/b)(1/a + 1/b)^t \sim \exp(-\kappa t)$. The conditional probability of being at a plateau of length $\varepsilon_k(t)$ at a given t is

$$P(k|t) = \frac{P(k, t)}{P(t)} = \frac{B(t, k)\varepsilon_k(t)}{\rho(t)} . \quad (2)$$

The characteristic plateau size is thus naturally chosen as $\tilde{\varepsilon}(t) = \varepsilon_{k^*}(t)$ where $k = k^*$ maximizes $P(k|t)$ in Eq. (2). Using Stirling's approximation we obtain $k^* \approx t/(1+b/a)$ and thus

$$\tilde{\varepsilon}(t) = \varepsilon_{k^*}(t) = \exp\left(-t \frac{a \log(b) + b \log(a)}{a + b}\right) . \quad (3)$$

In the context transient chaos, the construction of the Cantor set corresponds exactly to the escape time function of the one-dimensional open tent map [27] and the exponent $\lambda_L = \frac{a \log(b) + b \log(a)}{a + b}$ corresponds to its positive Lyapunov exponent [9]. This leads to a natural interpretation for a choice of $\sigma(t)$ with $\tilde{\varepsilon}(t)$ as given in Eq. (3): in order to ensure that two chaotic trajectories (initiated at r and r') remain correlated up to time t , their initial distance $|r - r'|$ should be reduced exponentially with t , with an exponent equal to the positive Lyapunov exponent responsible for the divergence in forward time. In a generic fractal landscape, generated by a higher dimensional system, this divergence is dominated by the maximal Lyapunov exponent λ_L and therefore

$$\sigma(t) \sim \tilde{\varepsilon}(t) \sim e^{-\lambda_L t} \quad (4)$$

should be used in any isotropic proposal such as Eq. (1).

S2 - Acceptance - Because of the extreme roughness of fractal landscapes, we use a flat-histogram simulation [1] on the variable t , which plays the role traditionally played by energy. The detailed balance of this Monte Carlo process is fulfilled when the acceptance, the conditional probability of accepting a proposed state \mathbf{r}' given \mathbf{r} , follows the Metropolis' choice [15]

$$A(\mathbf{r} \rightarrow \mathbf{r}') = \min \left\{ 1, \frac{\rho(t(\mathbf{r}')) g(\mathbf{r}' \rightarrow \mathbf{r})}{\rho(t(\mathbf{r})) g(\mathbf{r} \rightarrow \mathbf{r}')} \right\}, \quad (5)$$

where $g(\mathbf{r} \rightarrow \mathbf{r}')$ is given by Eqs. (1) and (4). Since we are considering projections in t , it is useful to define the conditional probability $A(t)$ of accepting a proposal given a time t [15]. In the spirit of flat-histogram simulations, a signature of an efficient random walk is a $A(t)$ which does not strongly depends on t . In Fig. 3 we show that only when the scaling in Eq. (4) is used in the Eq. (1), we obtain a constant $A(t)$ on a flat-histogram simulation in the generic 2-scale Cantor set and thus an efficient simulation.

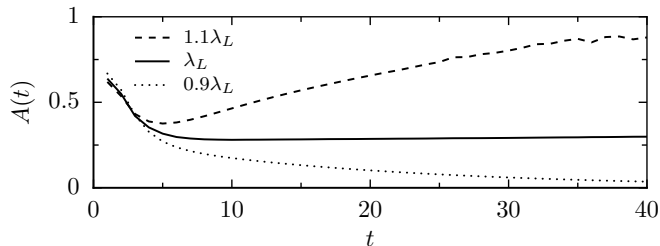


FIG. 3: Characteristic random-walk step σ has to scale as the typical plateau size $\tilde{\epsilon}$ in order to achieve a constant acceptance ratio in time. Acceptance ratio $A(t)$ of a flat-histogram simulation on the 2-scale Cantor set with parameters $(a, b) = (3, 4)$ and three (see legend) slightly different exponents λ on the proposal width $\sigma(t) \sim e^{-\lambda t}$, with λ_L given in Eq. (3). For $\lambda < \lambda_L$ and $t \gg 1$, $\sigma(t) \gg \tilde{\epsilon}(t)$, and $A(t)$ decays (exponentially) as a consequence of lack of proposals to $t' > t$. For $\lambda > \lambda_L$ and $t \gg 1$, $\sigma(t) \ll \tilde{\epsilon}(t)$, $A(t)$ increases to 1 but the simulation gets stuck in the same plateau as all proposals are for $t' = t$.

S3 - Wang-Landau update - In systems on which $\rho(t)$ and $\sigma(t)$ (or λ_L are known, we use steps **S1-S2** to sample them. However, for generic landscapes, $\rho(t)$ and $\sigma(t)$ are unknown. We take advantage of the analogy between $\rho(t)$ and a density of states and apply the Wang-Landau procedure to compute it [2]. This is done by successive approximating $\rho(t)$ in steps **S3** and **S4** of our approach. To compute $\sigma(t)$, we propose the following generalization of the Wang-Landau procedure (step **S3.1**) to the proposal distribution (step **S3.2**): if the proposed state has an escape time smaller than the present state, $t' < t$, we decrease $\sigma(t)$ by dividing it by f . If it has the same escape time, $t' = t$, we increase $\sigma(t)$ by multiplying it by f . This converges asymptotically ($f \rightarrow 1$) to a Markov process.

S4 - Refinement - In order to efficiently reduce the precision parameter f we take its square-root (as in Wang-Landau algorithm [2]) after a number of round-trips [15, 16], defined as the movement in the time-spectrum from t_{\min} to t_{\max} and back to t_{\min} , and we use an equivalent procedure to the one in Ref. [17] in order to avoid error saturation.

We now confirm the generality of the approach described above through numerical simulations in generic fractal landscapes generated by a family of N coupled Hénon maps on a ring

$$\begin{pmatrix} x_i \\ y_i \end{pmatrix} = \begin{pmatrix} A_i - x_i^2 + B y_i + k(x_i - x_{i+1}) \\ x_i \end{pmatrix}, \quad (6)$$

for $i = 1, \dots, N$, $N + 1 \equiv 1$, parameters $k = 0.4$, $B = 0.3$, $A_1 = 3$ (if $N > 1$), $A_N = 5$, and $A_i = A_1 + (A_N - A_1)(i - 1)/(N - 1)$. This choice of parameters ensures that a chaotic map is obtained in the $N = 1$ case and the map considered in Ref. [13] is recovered for $N = 2$ (used as a representative case to illustrate our algorithm). Initial conditions start on a $2N$ hypercube $\Gamma = [-4, 4]^{2N}$ and escape is defined as leaving Γ . In Fig. 4 we confirm the convergence and validity of our algorithm by showing that $\rho(t)$ coincides with uniform sampling, $\sigma(t)$ scales with the Lyapunov exponent reported in Ref. [13], and both the acceptance and the histogram of visits to escape time t are flat in t . We observed similar results for all N 's up to $N = 5$.

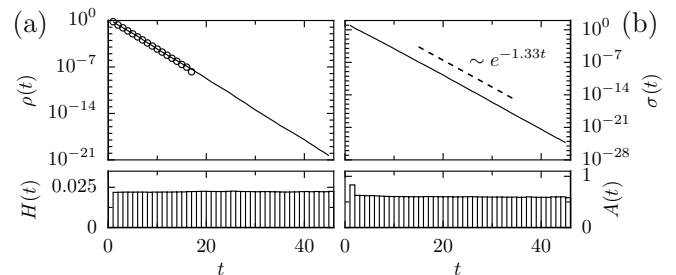


FIG. 4: (Color Online) Confirmation that our method yields the correct values of κ and λ_L and converges to a flat histogram simulation for the case $N = 2$ in Eq. (6). (a) $\rho(t)$ obtained through our method (line) and through uniform sampling (circles) with the exact same computational effort. Lower inset: histogram $H(t)$ of visits to escape times t . (b) $\sigma(t)$ obtained through our method. The dashed line shows the scaling $e^{-\lambda_L t}$ with $\lambda_L \approx 1.33$ obtained in Ref. [13]. Lower inset: the acceptance ratio $A(t)$. We used $[t_{\min}, t_{\max}] = [1, 45]$, $\log_e f_{\min} = 2^{-13}$ and all plotted quantities were measured on the last refinement.

We now compare our approach to uniform sampling in terms of computational efficiency. For each t_{\max} , we compute the average number of map iterations $n(t_{\max})$ per sampled state with $t = t_{\max}$. This comparison guarantees that the maximum uncertainty of any observable to be measured on the landscape is the same in both

cases for all $t \leq t_{\max}$. For a uniform-sampling simulation, $n(t_{\max}) \sim 1/\rho(t_{\max}) \sim e^{\kappa t_{\max}}$. For a flat-histogram simulation, obtained after the convergence of our method **S1-S4**, we adopt a conservative approach which avoids the sampling of correlated states by considering a single sample of t_{\max} for each round-trip. The estimation of $n(t_{\max})$ in this case is based on the number of steps per round-trip expected of an unbiased random walk with local steps ($\Delta t \approx 1$), which scales as $\sim t_{\max}^2$. Additionally, each proposal requires t map iterations and, since the histogram is flat, for each round trip one gets an additional t_{\max} contribution, leading to an expected scaling of $n \sim t_{\max}^3$. Figure 5 confirms the dramatic improve-

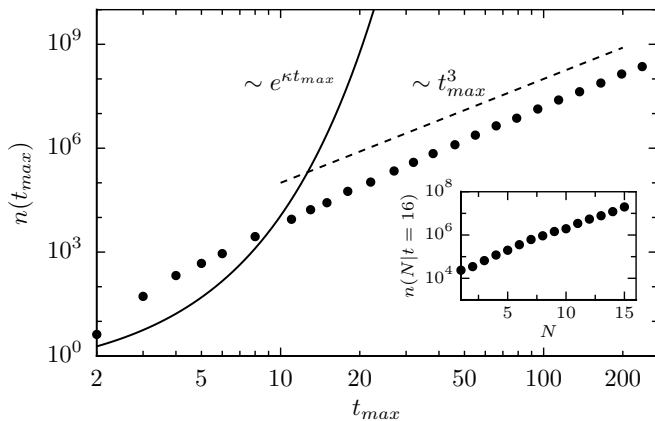


FIG. 5: The computation effort in number of map iterations $n(t_{\max})$ scales polynomially with maximum escape time, in contrast to the exponential scaling of uniform sampling. Main panel: results for uniform sampling (solid line) and flat-histogram simulation achieved by our method (squares) for the representative case $N = 4$ in Eq. (6). The dashed line indicates the scaling t_{\max}^3 . Inset: dependence of the efficiency on the phase-space dimension $2N$ at a fixed $t_{\max} = 16$.

ment from exponential (uniform sampling) to polynomial (our approach) scaling in the coupled Hénon maps. The significance of these results become apparent by noticing that $t_{\max} = 237$ (last point in Fig. 5) corresponds to $\rho(t_{\max}) \approx 10^{-109}$, meaning that we are able to sample extremely rare states. For such level of accuracy, our method requires an implementation with arbitrary precision [18] which in our case was able to resolve states which differ by 10^{-137} (since $\sigma(t_{\max} = 237) \approx 10^{-137}$). Interestingly, the slight but clear deviation from the prediction t_{\max}^3 seen in Fig. 5 shows that flat-histogram simulations on fractal landscapes are not purely diffusive on t , a phenomenon known in spin-systems as critical slowing down [19, 20]. This phenomenon is enhanced with increasing dimension and contributes to the exponential increase of n_{\max} with N for a fixed t_{\max} , as shown in the inset of Fig. 5. Still, a uniform sampling in such a high phase-space dimension ($2N = 30$) would need impracticable $n \approx 10^{34}$ map iterations to sample one state with $t_{\max} = 16$.

In summary, we have shown how flat-histogram Monte Carlo simulations can be performed on fractal landscapes. The crucial ingredient is to consider a random-walk step size dependent on the height of the landscape. The correct dependency should scale as the characteristic length of the landscape and can be obtained through an adaptive procedure which generalizes Wang-Landau's algorithm to the proposal distribution. This idea can find applications in any rough landscape for which there is a typical width at a fixed height and a strong dependence with the height. Fractality can be considered as an extreme case of roughness which naturally occurs in the escape-time landscape of open chaotic systems. In this case, our results show that the Lyapunov exponent λ_L , a fundamental property of the chaotic dynamics, is an essential ingredient for a flat-histogram simulation.

We emphasize the significance of our results for numerical investigations of open chaotic systems. Our method automatically provides κ and λ_L , is not limited to low dimension, and allows for the computation of expected values of any observable using a flat-histogram simulation. For the specific problem of finding the chaotic saddle [12–14], which is indirectly solved in our simulations by storing trajectories with large t , our findings show that best results are achieved using a proposal which scales as $e^{-\lambda_L t}$.

More generally, besides high-dimensionality, the sensitivity of initial conditions in chaotic systems is a major reason for using statistical methods in physics. Monte Carlos methods in dynamical systems were traditionally limited to uniform sampling and, only recently, optimized methods (with non-uniform sampling) were applied for the problem of finding trajectories with low chaoticity [21, 22]. Our approach opens the perspective of using the full strength of optimized Monte Carlo methods to problems which involve the computation of averages in chaotic systems. Spatially extended [23] and non-hyperbolic Hamiltonian [24] systems are natural candidates for future applications of this approach.

We are indebted to T. Tél and P. Grassberger for insightful discussions. J.C.L. acknowledges funding from Erasmus 29233-IC-1-2007-1-PT-ERASMUS-EUCX-1 and Max Planck Society.

* jleita@pks.mpg.de

† jvlopes@fe.up.pt

‡ edugalt@pks.mpg.de

- [1] B. A. Berg and T. Neuhaus, Phys. Lett. B **267**, 249 (1991).
- [2] F. Wang and D. Landau, Phys. Rev. Lett. **86**, 2050 (2001).
- [3] J. Viana Lopes, M. Costa, J. dos Santos, and R. Toral, Phys. Rev. E **74**, 046702 (2006).
- [4] R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **57**,

- 2607 (1986).
- [5] Q. Yan and J. de Pablo, Phys. Rev. Lett. **90**, 035701 (2003).
 - [6] S. Trebst, M. Troyer, and U. H. E. Hansmann, J. Chem. Phys. **124**, 174903 (2006).
 - [7] P. Grassberger, Phys. Rev. E **56**, 3682 (1997).
 - [8] E. Ott, *Chaos in Dynamical Systems*, 2nd ed. (Cambridge University Press, Cambridge, 1993).
 - [9] Y.-C. Lai and T. Tél, *Transient chaos: Complex dynamics in finite time scales*, 1st ed., edited by S. S. Antman, J. E. Marsden, and L. Sirovich, Vol. 173 (Springer, New York, 2010).
 - [10] E. G. Altmann, J. S. E. Portela, and T. Tél, arXiv 1208.0254v2 (2013).
 - [11] A. P. S. de Moura and C. Grebogi, Phys. Rev. Lett. **86**, 2778 (2001).
 - [12] H. E. Nusse and J. A. Yorke, Physica D **36**, 137 (1989).
 - [13] D. Sweet, H. E. Nusse, and J. A. Yorke, Phys. Rev. Lett. **86**, 2261 (2001).
 - [14] E. M. Bollt, Int. J. Bifurcat. Chaos **15**, 1615 (2005).
 - [15] M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics* (Oxford University Press, USA, New York, 2002).
 - [16] M. D. Costa, J. Viana Lopes, and J. M. B. L. dos Santos, Europhys. Lett. **72**, 802 (2007).
 - [17] R. Belardinelli and V. Pereyra, Phys. Rev. E **75**, 046701 (2007).
 - [18] T. Granlund and the GMP Development Team, “GNU MP,” (2012).
 - [19] P. Dayal, S. Trebst, S. Wessel, D. Wurtz, M. Troyer, S. Sabhapandit, and S. N. Coppersmith, Phys. Rev. Lett. **92**, 097201 (2004).
 - [20] S. Trebst, D. A. Huse, and M. Troyer, Phys. Rev. E **70**, 046701 (2004).
 - [21] T. Yanagita and Y. Iba, J. Stat. Mech.-Theory E, P02043 (2009).
 - [22] J. Tailleur and J. Kurchan, Nat. Phys. **3**, 203 (2007).
 - [23] T. Tél and Y.-C. Lai, Phys. Rep. **460**, 245 (2008).
 - [24] G. Cristadoro and R. Ketzmerick, Phys. Rev. Lett. **100**, 184101 (2008).
 - [25] which intersects the stable manifold of the chaotic saddle
 - [26] we have checked that a normal distribution instead of exponential distribution with standard deviation $\sigma(t)$ gives equivalent results.
 - [27] The tent map is defined on $x \in [0, 1]$ as $x_{t+1} = ax_t$ for $x_t < b/(a+b)$ and $x_{t+1} = b(1-x_t)$ for $x_t > b/(a+b)$ [9].